



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:40 PM UTC

PDB ID : 3FZ6 / pdb_00003fz6
Title : Crystal structure of glutamate decarboxylase beta from Escherichia coli: complex with xenon
Authors : Malashkevich, V.N.; De Biase, D.; Bossa, F.
Deposited on : 2009-01-23
Resolution : 2.82 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

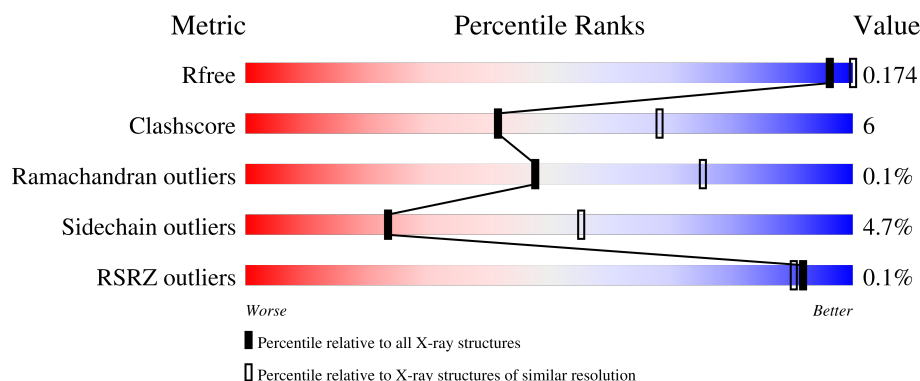
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	466	
1	B	466	
1	C	466	
1	D	466	
1	E	466	

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Mol	Chain	Length	Quality of chain
1	F	466	 82% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PMP	D	500	-	-	X	-
2	PMP	E	500	-	-	X	-

2 Entry composition [i](#)

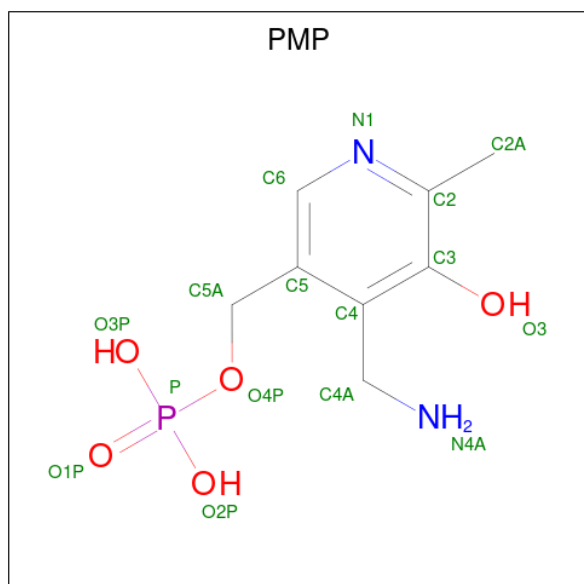
There are 4 unique types of molecules in this entry. The entry contains 22347 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate decarboxylase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	2	0
			3636	2325	618	669	24			
1	B	463	Total	C	N	O	S	0	1	0
			3690	2355	630	681	24			
1	C	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			
1	D	455	Total	C	N	O	S	0	1	0
			3625	2316	617	668	24			
1	E	464	Total	C	N	O	S	0	1	0
			3699	2361	632	682	24			
1	F	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: C₈H₁₃N₂O₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	E	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	F	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 3 is XENON (CCD ID: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Xe	0	0
			1	1		
3	B	1	Total	Xe	0	0
			1	1		
3	C	1	Total	Xe	0	0
			1	1		
3	D	1	Total	Xe	0	0
			1	1		
3	E	1	Total	Xe	0	0
			1	1		
3	F	1	Total	Xe	0	0
			1	1		

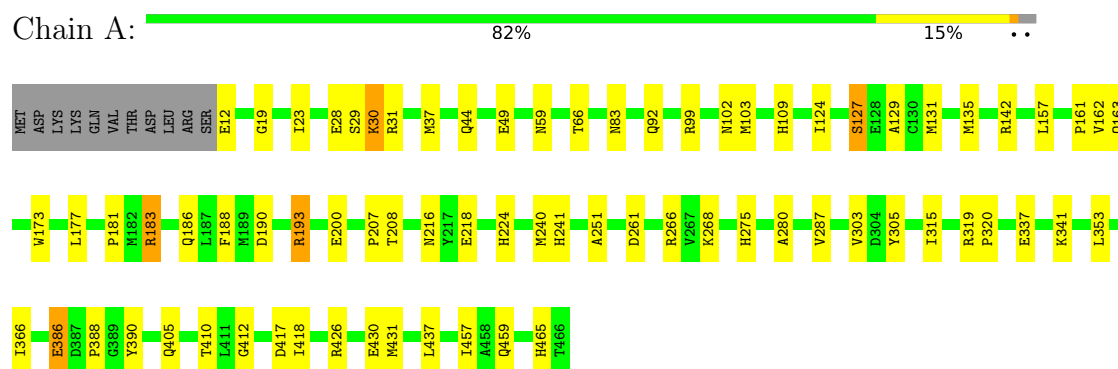
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	363	Total	O	0	0
			363	363		

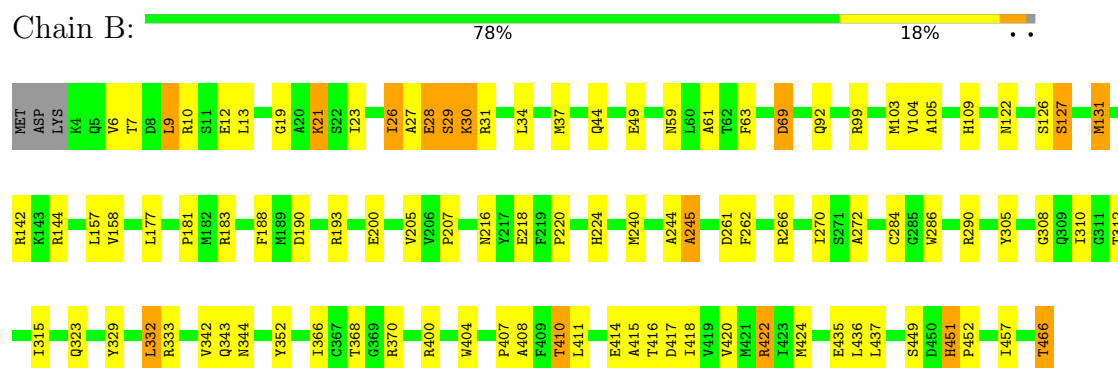
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

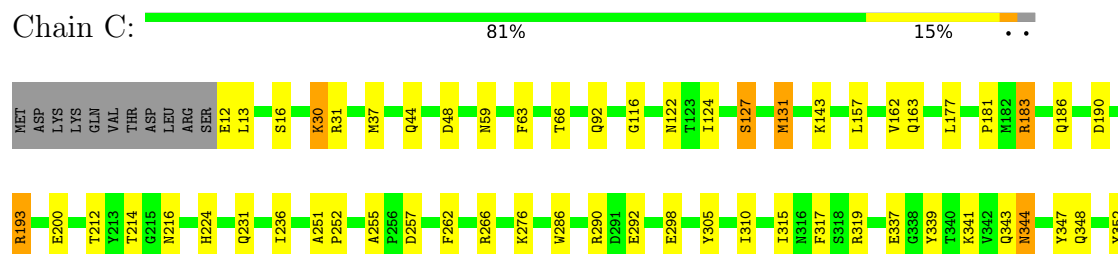
- Molecule 1: Glutamate decarboxylase beta



- Molecule 1: Glutamate decarboxylase beta



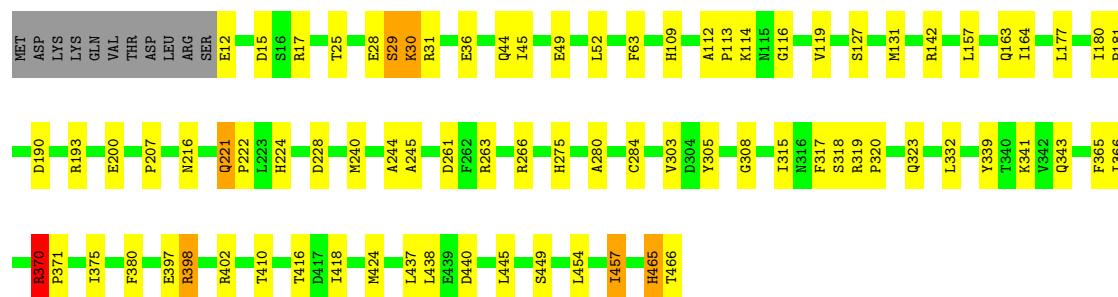
- Molecule 1: Glutamate decarboxylase beta





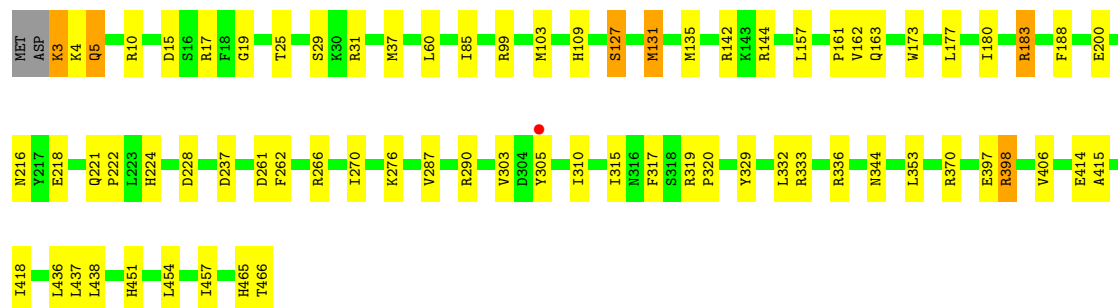
• Molecule 1: Glutamate decarboxylase beta

Chain D: 80% 16% ..



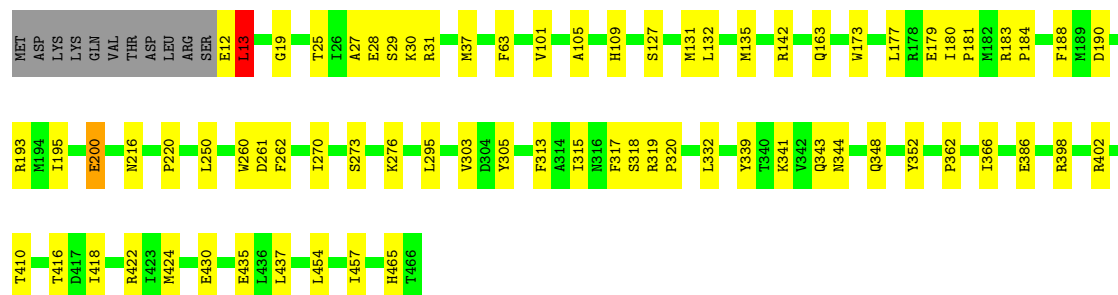
• Molecule 1: Glutamate decarboxylase beta

Chain E: 84% 14% .



• Molecule 1: Glutamate decarboxylase beta

Chain F: 82% 15% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	116.73Å 116.73Å 208.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.85 – 2.82 19.85 – 2.82	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.85-2.82) 97.9 (19.85-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.83Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.135 , 0.203 (Not available) , 0.174	Depositor DCC
R_{free} test set	3768 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.030 for h,-h-k,-l 0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22347	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PMP, XE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.88	0/3735	1.06	9/5062 (0.2%)
1	B	0.89	0/3788	1.05	5/5133 (0.1%)
1	C	0.95	0/3710	1.08	6/5028 (0.1%)
1	D	0.92	1/3723 (0.0%)	1.06	8/5046 (0.2%)
1	E	0.98	2/3797 (0.1%)	1.05	5/5144 (0.1%)
1	F	0.95	3/3710 (0.1%)	1.04	5/5028 (0.1%)
All	All	0.93	6/22463 (0.0%)	1.06	38/30441 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	317	PHE	CA-C	9.96	1.57	1.52
1	D	317	PHE	CA-C	8.59	1.56	1.52
1	F	317	PHE	CA-C	7.20	1.56	1.52
1	F	250	LEU	CA-C	-5.65	1.49	1.52
1	F	105	ALA	CA-CB	-5.07	1.45	1.53
1	E	85	ILE	CA-CB	5.04	1.60	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	162	VAL	CB-CA-C	-8.29	102.17	111.45
1	A	29	SER	N-CA-C	-6.62	104.42	113.30
1	A	102	ASN	N-CA-C	6.57	118.44	111.28
1	B	26	ILE	N-CA-C	6.25	116.40	110.53
1	D	29	SER	N-CA-C	-6.23	105.26	112.92
1	B	451	HIS	CA-C-N	6.12	125.81	119.56
1	B	451	HIS	C-N-CA	6.12	125.81	119.56
1	B	457	ILE	N-CA-C	5.92	115.98	110.42
1	F	101	VAL	N-CA-C	-5.87	104.79	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	344	ASN	N-CA-C	5.87	118.43	111.33
1	F	30	LYS	N-CA-C	-5.80	106.24	113.55
1	D	375	ILE	CA-C-N	-5.73	112.68	119.84
1	D	375	ILE	C-N-CA	-5.73	112.68	119.84
1	E	37	MET	N-CA-C	-5.70	100.04	108.99
1	D	457	ILE	N-CA-C	5.60	115.80	110.53
1	E	451	HIS	CA-C-N	5.56	125.23	119.56
1	E	451	HIS	C-N-CA	5.56	125.23	119.56
1	D	119	VAL	CB-CA-C	-5.54	105.93	111.80
1	A	162	VAL	CB-CA-C	-5.54	105.50	111.59
1	A	251	ALA	CA-C-N	-5.49	113.96	119.56
1	A	251	ALA	C-N-CA	-5.49	113.96	119.56
1	C	428	GLY	N-CA-C	-5.36	107.85	113.58
1	C	48	ASP	N-CA-C	5.35	117.81	111.33
1	F	37	MET	N-CA-C	-5.32	100.64	108.99
1	C	37	MET	N-CA-C	-5.24	101.10	109.07
1	A	83	ASN	N-CA-C	5.22	116.82	108.41
1	A	241	HIS	CA-C-N	-5.22	116.35	122.93
1	A	241	HIS	C-N-CA	-5.22	116.35	122.93
1	C	13	LEU	N-CA-C	5.21	117.25	109.59
1	B	422	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	F	105	ALA	N-CA-C	-5.10	105.61	111.07
1	C	66	THR	N-CA-C	-5.09	106.20	114.09
1	A	457	ILE	N-CA-C	5.09	115.31	110.53
1	D	465	HIS	N-CA-C	5.07	119.46	113.28
1	E	162	VAL	CB-CA-C	-5.04	106.05	111.59
1	F	13	LEU	N-CA-C	5.03	117.60	110.10
1	D	370	ARG	CA-C-N	5.02	124.80	119.28
1	D	370	ARG	C-N-CA	5.02	124.80	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3636	0	3533	44	0
1	B	3690	0	3595	57	0
1	C	3616	0	3516	52	0
1	D	3625	0	3525	53	0
1	E	3699	0	3608	47	0
1	F	3616	0	3516	50	0
2	A	16	0	11	2	0
2	B	16	0	11	5	0
2	C	16	0	11	5	0
2	D	16	0	11	7	0
2	E	16	0	11	6	0
2	F	16	0	11	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	E	363	0	0	10	0
All	All	22347	0	21359	279	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (279) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:500:PMP:HNA1	2:B:500:PMP:H5A1	0.97	1.09
2:B:500:PMP:HNA1	2:B:500:PMP:C5A	1.63	1.04
1:D:163:GLN:HG3	2:D:500:PMP:HNA1	1.23	1.02
1:E:305[A]:TYR:HE1	1:E:310:ILE:HG13	1.28	0.97
1:E:305[A]:TYR:CE1	1:E:310:ILE:HG13	2.03	0.93
2:B:500:PMP:H5A1	2:B:500:PMP:N4A	1.82	0.92
1:C:190:ASP:OD1	1:C:193:ARG:HD3	1.75	0.87
1:C:163:GLN:HG3	2:C:500:PMP:HNA1	1.40	0.85
1:A:59:ASN:O	1:A:426:ARG:NH2	2.12	0.82
1:C:30:LYS:HE3	1:D:116:GLY:O	1.81	0.80
1:F:190:ASP:OD1	1:F:193:ARG:HD3	1.82	0.80
1:F:303:VAL:HG23	1:F:305:TYR:CE1	2.16	0.79
2:B:500:PMP:C5A	2:B:500:PMP:N4A	2.43	0.77
1:E:303:VAL:HG23	1:E:305[B]:TYR:CE2	2.20	0.76
1:B:352:TYR:OH	1:B:435:GLU:OE1	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:THR:O	1:B:370:ARG:NH2	2.18	0.76
1:B:27:ALA:O	1:B:28:GLU:HB2	1.85	0.76
1:E:465:HIS:ND1	4:E:804:HOH:O	2.11	0.74
1:C:131:MET:CE	1:D:315:ILE:HG23	2.18	0.73
1:D:190:ASP:OD1	1:D:193:ARG:HD3	1.87	0.73
1:A:188[A]:PHE:HZ	1:A:216:ASN:HD22	1.32	0.73
1:F:465:HIS:O	2:F:500:PMP:N4A	2.23	0.71
1:D:163:GLN:CG	2:D:500:PMP:HNA1	2.00	0.70
1:A:99:ARG:HD3	1:B:29:SER:HB2	1.71	0.70
1:E:127:SER:O	1:E:131:MET:HG2	1.91	0.70
1:D:12:GLU:HB2	4:E:818:HOH:O	1.92	0.69
1:E:144:ARG:NH2	4:E:667:HOH:O	2.24	0.69
1:C:466:THR:HG23	1:C:466:THR:OXT	1.91	0.68
1:B:19:GLY:O	1:C:341:LYS:HE3	1.94	0.68
1:C:131:MET:HE3	1:D:315:ILE:HG23	1.75	0.67
1:C:183:ARG:HG3	1:C:186:GLN:HB3	1.76	0.66
1:E:415:ALA:HB1	1:E:418:ILE:HD12	1.76	0.66
1:E:163:GLN:HG3	2:E:500:PMP:C4	2.26	0.66
1:D:181:PRO:O	1:D:193:ARG:NH2	2.30	0.65
1:E:25:THR:O	1:E:29:SER:HB3	1.97	0.65
1:C:30:LYS:CE	1:D:116:GLY:O	2.45	0.64
1:A:181:PRO:O	1:A:193:ARG:NH2	2.31	0.64
1:C:415:ALA:HB1	1:C:418:ILE:HD12	1.78	0.64
1:E:144:ARG:CZ	4:E:667:HOH:O	2.46	0.64
1:A:190:ASP:OD1	1:A:193:ARG:HD3	1.97	0.64
1:B:190:ASP:OD1	1:B:193:ARG:HD3	1.96	0.64
1:E:303:VAL:HG23	1:E:305[B]:TYR:HE2	1.61	0.63
1:A:386:GLU:HG3	4:E:673:HOH:O	1.97	0.63
1:B:343:GLN:HA	1:B:343:GLN:OE1	1.98	0.63
1:B:23:ILE:HG21	1:B:37:MET:HE2	1.81	0.62
1:A:341:LYS:HE3	1:F:19:GLY:O	2.00	0.61
1:E:319:ARG:HB2	1:E:320:PRO:HD2	1.82	0.61
1:C:305:TYR:HE1	1:C:310:ILE:HG13	1.64	0.61
1:D:305[A]:TYR:CD1	1:D:308:GLY:O	2.53	0.61
1:A:49:GLU:O	1:B:92:GLN:HG2	2.00	0.61
1:E:131:MET:HE3	1:F:315:ILE:HG23	1.81	0.61
1:C:214:THR:OG1	1:C:216:ASN:ND2	2.33	0.60
1:A:465:HIS:O	2:A:500:PMP:N4A	2.35	0.60
1:C:116:GLY:O	1:D:30:LYS:HE2	2.02	0.59
1:D:25:THR:O	1:D:29:SER:HB3	2.02	0.59
1:F:352:TYR:OH	1:F:435:GLU:OE1	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:303:VAL:HG23	1:F:305:TYR:HE1	1.66	0.59
1:F:362:PRO:HB2	1:F:386:GLU:HG2	1.85	0.59
1:F:63:PHE:CD2	1:F:424:MET:HE2	2.39	0.58
2:E:500:PMP:C5A	2:E:500:PMP:N4A	2.67	0.58
1:F:135:MET:HE2	1:F:173:TRP:CZ2	2.39	0.58
1:D:216:ASN:HD21	1:D:366:ILE:HG22	1.67	0.58
1:A:224:HIS:CD2	1:A:266:ARG:HB2	2.39	0.57
1:F:25:THR:O	1:F:29:SER:HB3	2.03	0.57
1:B:109:HIS:HD2	1:B:261:ASP:OD2	1.86	0.57
1:D:303:VAL:HG23	1:D:305[B]:TYR:CE2	2.40	0.57
1:D:63:PHE:CD2	1:D:424:MET:HE2	2.40	0.57
1:A:19:GLY:O	1:F:341:LYS:HE3	2.05	0.56
1:B:158:VAL:HB	1:B:205:VAL:HG22	1.87	0.56
1:B:181:PRO:O	1:B:193:ARG:NH2	2.39	0.56
1:C:163:GLN:CG	2:C:500:PMP:HNA1	2.13	0.56
1:C:181:PRO:O	1:C:193:ARG:NH2	2.37	0.56
1:F:127:SER:O	1:F:131:MET:HG2	2.05	0.56
1:A:303:VAL:HG23	1:A:305[B]:TYR:CE2	2.40	0.56
1:A:37:MET:HE1	1:B:332:LEU:HD22	1.86	0.56
1:C:131:MET:HE2	1:D:315:ILE:HG23	1.86	0.56
1:A:207:PRO:HG3	1:A:240:MET:HE2	1.88	0.56
1:E:3:LYS:C	1:E:5:GLN:H	2.14	0.56
1:A:431:MET:HE3	1:F:13:LEU:HG	1.89	0.55
1:B:27:ALA:O	1:B:28:GLU:CB	2.53	0.55
1:A:315:ILE:HG23	1:B:131:MET:HE3	1.88	0.55
1:B:12:GLU:OE1	1:B:21:LYS:NZ	2.39	0.55
1:A:127:SER:O	1:A:131:MET:HG2	2.07	0.55
1:D:15:ASP:OD1	1:D:17:ARG:HB2	2.07	0.55
1:F:276:LYS:NZ	2:F:500:PMP:H4A2	2.21	0.55
1:A:319:ARG:HB2	1:A:320:PRO:HD2	1.89	0.54
1:D:163:GLN:NE2	1:D:164:ILE:HG22	2.21	0.54
1:E:228:ASP:HA	1:E:266:ARG:HH21	1.72	0.54
1:D:224:HIS:CD2	1:D:266:ARG:HB2	2.43	0.54
1:A:12:GLU:CD	1:A:12:GLU:N	2.65	0.54
1:E:224:HIS:CD2	1:E:266:ARG:HB2	2.42	0.54
1:C:317:PHE:O	1:C:319:ARG:HG2	2.08	0.54
1:E:262:PHE:CE2	1:E:270:ILE:HD12	2.43	0.53
1:E:329:TYR:CZ	1:E:333:ARG:HD3	2.43	0.53
1:A:66:THR:OG1	1:A:426:ARG:NH1	2.42	0.53
1:C:63:PHE:HB3	1:C:276:LYS:HG2	1.91	0.53
1:C:344:ASN:O	1:C:348:GLN:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188[A]:PHE:HZ	1:A:216:ASN:ND2	2.03	0.53
1:A:188[A]:PHE:CZ	1:A:216:ASN:ND2	2.77	0.53
1:D:465:HIS:O	2:D:500:PMP:N4A	2.35	0.52
1:C:224:HIS:CD2	1:C:266:ARG:HB2	2.43	0.52
1:C:410:THR:HA	1:C:418:ILE:O	2.09	0.52
1:F:177:LEU:CD1	1:F:179:GLU:HB2	2.39	0.52
1:C:122:ASN:HB2	1:C:286:TRP:CZ3	2.44	0.52
1:B:224:HIS:CD2	1:B:266:ARG:HB2	2.44	0.52
1:F:402:ARG:HG2	1:F:402:ARG:HH11	1.75	0.52
1:F:410:THR:HA	1:F:418:ILE:O	2.10	0.52
1:C:387:ASP:OD1	1:C:387:ASP:C	2.52	0.51
1:C:292:GLU:OE2	4:E:534:HOH:O	2.19	0.51
1:C:212:THR:O	1:C:422:ARG:NH1	2.42	0.51
1:F:303:VAL:CG2	1:F:305:TYR:CE1	2.91	0.51
1:E:221:GLN:HB3	1:E:222:PRO:HD3	1.93	0.51
1:D:339:TYR:O	1:D:343:GLN:HG2	2.11	0.51
1:C:63:PHE:CD1	1:C:466:THR:HA	2.46	0.50
1:E:60:LEU:HD12	1:E:406:VAL:HG22	1.93	0.50
1:D:163:GLN:HG3	2:D:500:PMP:N4A	2.07	0.50
1:E:183:ARG:HB3	1:E:414:GLU:HB2	1.93	0.50
1:F:295:LEU:HD11	1:F:313:PHE:CD2	2.46	0.50
1:F:319:ARG:HB2	1:F:320:PRO:HD2	1.92	0.50
1:A:275:HIS:HA	1:A:280:ALA:O	2.12	0.49
1:E:109:HIS:HD2	1:E:261:ASP:OD2	1.95	0.49
1:B:216:ASN:HD21	1:B:366:ILE:HG22	1.76	0.49
1:E:221:GLN:O	1:E:222:PRO:C	2.54	0.49
1:B:122:ASN:HB2	1:B:286:TRP:CZ3	2.48	0.49
1:C:163:GLN:HG3	2:C:500:PMP:N4A	2.20	0.49
1:F:163:GLN:HG3	2:F:500:PMP:C4	2.42	0.49
1:B:218:GLU:O	1:B:220:PRO:HD3	2.13	0.49
1:F:109:HIS:HD2	1:F:261:ASP:OD2	1.95	0.49
1:B:262:PHE:CE2	1:B:270:ILE:HD12	2.48	0.49
1:A:129:ALA:HB1	1:A:287:VAL:HB	1.95	0.48
1:C:411:LEU:O	1:C:416:THR:HA	2.12	0.48
2:E:500:PMP:C5A	2:E:500:PMP:HNA1	2.24	0.48
1:A:465:HIS:ND1	4:E:807:HOH:O	2.24	0.48
1:B:245:ALA:HA	1:B:272:ALA:HA	1.95	0.48
1:F:177:LEU:HD12	1:F:179:GLU:HB2	1.96	0.48
1:F:181:PRO:O	1:F:193:ARG:NH2	2.44	0.48
1:C:465:HIS:O	1:C:466:THR:HB	2.13	0.48
1:D:402:ARG:HD3	1:D:440:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:PHE:O	1:B:290:ARG:NH2	2.47	0.47
1:C:12:GLU:OE2	1:C:12:GLU:HA	2.14	0.47
1:E:144:ARG:NE	4:E:667:HOH:O	2.48	0.47
1:B:26:ILE:O	1:B:29:SER:HB3	2.15	0.47
1:B:61:ALA:HB2	1:B:407:PRO:HD3	1.97	0.47
1:B:104:VAL:O	1:B:105:ALA:C	2.56	0.47
1:D:221:GLN:HB3	1:D:222:PRO:HD3	1.95	0.47
1:B:466:THR:OXT	1:B:466:THR:HG23	2.14	0.47
1:D:261:ASP:CG	1:D:263:ARG:HH21	2.23	0.47
1:A:410:THR:HA	1:A:418:ILE:O	2.15	0.47
1:A:216:ASN:HD21	1:A:366:ILE:HG22	1.79	0.47
1:A:23:ILE:HG21	1:A:37:MET:HE2	1.97	0.46
1:B:19:GLY:O	1:C:341:LYS:CE	2.63	0.46
1:B:224:HIS:NE2	1:B:266:ARG:HB2	2.30	0.46
1:C:353:LEU:HD23	1:C:353:LEU:HA	1.69	0.46
1:C:59:ASN:OD1	1:C:59:ASN:C	2.58	0.46
1:F:339:TYR:O	1:F:343:GLN:HG2	2.16	0.46
1:B:9:LEU:HD21	1:C:371:PRO:HG2	1.96	0.46
1:B:305[A]:TYR:CD1	1:B:308:GLY:O	2.69	0.46
1:E:466:THR:HG21	1:F:318:SER:OG	2.16	0.46
1:A:135:MET:HE2	1:A:173:TRP:CZ2	2.50	0.46
1:B:343:GLN:OE1	1:B:343:GLN:CA	2.63	0.46
1:E:135:MET:HE2	1:E:173:TRP:CZ2	2.51	0.46
1:F:183:ARG:O	1:F:184:PRO:C	2.59	0.46
1:A:109:HIS:HD2	1:A:261:ASP:OD2	1.98	0.46
1:F:132:LEU:HD22	1:F:313:PHE:CE1	2.51	0.46
1:B:411:LEU:O	1:B:416:THR:HA	2.16	0.46
2:E:500:PMP:N4A	2:E:500:PMP:H5A1	2.31	0.46
1:B:408:ALA:HA	1:B:420:VAL:O	2.17	0.45
1:E:303:VAL:CG2	1:E:305[B]:TYR:CE2	2.95	0.45
1:E:336:ARG:HD3	4:E:726:HOH:O	2.15	0.45
1:C:262:PHE:O	1:C:290:ARG:NH2	2.49	0.45
1:B:63:PHE:CD2	1:B:424:MET:HE2	2.51	0.45
1:D:112:ALA:HA	1:D:113:PRO:HD3	1.84	0.45
1:F:362:PRO:CB	1:F:386:GLU:HG2	2.47	0.45
1:B:284:CYS:HB2	1:B:323:GLN:HB3	1.99	0.45
1:B:305[A]:TYR:CE1	1:B:310:ILE:HG13	2.52	0.45
1:C:92:GLN:HG2	1:D:49:GLU:O	2.16	0.45
1:C:352:TYR:OH	1:C:435:GLU:OE1	2.23	0.45
1:D:341:LYS:HE3	1:E:19:GLY:O	2.17	0.45
1:F:276:LYS:CE	2:F:500:PMP:H4A2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ARG:HB3	1:B:414:GLU:HB2	1.97	0.45
4:E:558:HOH:O	1:F:430:GLU:HB3	2.17	0.45
2:C:500:PMP:O2P	1:D:318:SER:HB2	2.17	0.45
1:D:163:GLN:HG3	2:D:500:PMP:C4	2.46	0.45
1:D:228:ASP:HA	1:D:266:ARG:HH21	1.82	0.45
1:C:400:ARG:HA	1:C:404:TRP:O	2.17	0.45
1:A:337:GLU:O	1:A:341:LYS:HD3	2.17	0.44
1:A:131:MET:HE3	1:B:315:ILE:HG23	1.99	0.44
1:B:99:ARG:HB3	1:B:103:MET:HE3	2.00	0.44
1:E:315:ILE:HG21	1:F:315:ILE:HG21	1.98	0.44
1:A:388:PRO:HB2	1:A:390:TYR:CE2	2.53	0.44
1:D:207:PRO:HG3	1:D:240:MET:HE2	1.98	0.44
1:A:183:ARG:NH1	1:A:186:GLN:OE1	2.51	0.44
1:B:400:ARG:HA	1:B:404:TRP:O	2.18	0.44
1:C:63:PHE:CD2	1:C:424:MET:HE2	2.53	0.44
1:E:353:LEU:HD23	1:E:353:LEU:HA	1.88	0.44
1:D:109:HIS:HD2	1:D:261:ASP:OD2	2.01	0.44
1:F:220:PRO:HG2	1:F:260:TRP:HB2	1.99	0.44
1:F:454:LEU:HA	1:F:457:ILE:HD12	2.00	0.44
1:D:319:ARG:HB2	1:D:320:PRO:HD2	2.00	0.44
1:B:126:SER:HB2	2:B:500:PMP:O4P	2.18	0.43
1:D:163:GLN:HG3	2:D:500:PMP:C3	2.48	0.43
1:E:99:ARG:HG2	1:F:29:SER:HB2	2.00	0.43
1:D:397:GLU:CD	1:E:398:ARG:HH22	2.26	0.43
1:E:237:ASP:OD1	1:E:266:ARG:NH1	2.51	0.43
1:D:52:LEU:HD23	1:D:52:LEU:HA	1.79	0.43
1:A:59:ASN:HA	1:A:405:GLN:HB3	2.01	0.43
1:B:415:ALA:C	1:B:417:ASP:H	2.27	0.43
1:E:131:MET:HG2	1:E:131:MET:H	1.63	0.43
1:F:195:ILE:HD13	1:F:195:ILE:HA	1.92	0.43
1:B:69:ASP:OD1	1:B:69:ASP:C	2.62	0.43
1:D:45:ILE:O	1:D:49:GLU:HG3	2.19	0.43
1:D:454:LEU:HD23	1:D:454:LEU:HA	1.93	0.43
1:E:161:PRO:HD2	1:E:218:GLU:OE2	2.19	0.43
1:F:200:GLU:H	1:F:200:GLU:HG3	1.59	0.43
1:B:127:SER:O	1:B:131:MET:HG2	2.18	0.42
1:C:347:TYR:CE1	1:C:371:PRO:HA	2.53	0.42
1:B:329:TYR:CZ	1:B:333:ARG:HD3	2.55	0.42
1:B:451:HIS:N	1:B:452:PRO:HD3	2.33	0.42
1:D:163:GLN:HB2	2:D:500:PMP:C2	2.48	0.42
1:D:454:LEU:HA	1:D:457:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:ASP:OD1	1:E:17:ARG:HB2	2.20	0.42
1:E:465:HIS:O	2:E:500:PMP:H4A2	2.19	0.42
1:D:28:GLU:O	1:D:28:GLU:HG2	2.19	0.42
1:D:275:HIS:HA	1:D:280:ALA:O	2.19	0.42
1:D:365:PHE:CD2	1:D:380:PHE:HB3	2.54	0.42
1:E:99:ARG:HD3	1:F:29:SER:HB2	2.01	0.42
1:F:402:ARG:HG2	1:F:402:ARG:NH1	2.33	0.42
1:F:343:GLN:OE1	1:F:343:GLN:HA	2.19	0.42
1:A:207:PRO:CG	1:A:240:MET:HE2	2.49	0.42
1:B:207:PRO:HG2	1:B:240:MET:HE2	2.02	0.42
1:D:303:VAL:HG23	1:D:305[B]:TYR:HE2	1.83	0.42
1:F:27:ALA:O	1:F:28:GLU:HB3	2.19	0.42
1:F:422:ARG:HE	1:F:422:ARG:HB3	1.54	0.42
1:C:339:TYR:O	1:C:343:GLN:HG2	2.19	0.42
1:C:395:LEU:HD21	1:C:441:TYR:CZ	2.54	0.42
1:F:273:SER:HB2	1:F:276:LYS:HD2	2.01	0.42
1:A:92:GLN:HG2	1:B:49:GLU:O	2.20	0.42
1:C:127:SER:O	1:C:131:MET:HG2	2.19	0.42
1:D:465:HIS:O	1:D:466:THR:HB	2.19	0.42
1:A:353:LEU:HD23	1:A:353:LEU:HA	1.86	0.41
1:B:30:LYS:HD2	1:B:30:LYS:HA	1.74	0.41
1:C:251:ALA:N	1:C:252:PRO:CD	2.83	0.41
1:D:410:THR:HA	1:D:418:ILE:O	2.21	0.41
1:E:188:PHE:HZ	1:E:216:ASN:HD22	1.68	0.41
1:C:143:LYS:HE2	1:C:298:GLU:OE1	2.20	0.41
1:E:454:LEU:HA	1:E:457:ILE:HD12	2.02	0.41
1:F:188:PHE:HZ	1:F:216:ASN:ND2	2.18	0.41
1:A:161:PRO:HD2	1:A:218:GLU:OE2	2.20	0.41
1:D:244:ALA:O	1:D:245:ALA:C	2.63	0.41
1:E:262:PHE:O	1:E:290:ARG:NH2	2.52	0.41
1:F:216:ASN:HD21	1:F:366:ILE:HG22	1.84	0.41
1:C:231:GLN:HB2	1:C:236:ILE:O	2.21	0.41
1:F:344:ASN:O	1:F:348:GLN:HG3	2.20	0.41
1:A:208:THR:O	1:A:218:GLU:HB2	2.20	0.41
1:B:188:PHE:HZ	1:B:216:ASN:HD22	1.69	0.41
1:B:244:ALA:O	1:B:245:ALA:C	2.64	0.41
1:A:30:LYS:HD3	1:A:30:LYS:HA	1.87	0.41
1:A:430:GLU:O	1:A:431:MET:C	2.64	0.41
1:B:59:ASN:OD1	1:B:59:ASN:C	2.63	0.41
1:F:188:PHE:CZ	1:F:216:ASN:ND2	2.89	0.41
1:D:398:ARG:HH22	1:E:397:GLU:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:GLN:O	1:E:224:HIS:N	2.53	0.41
1:E:438:LEU:HD23	1:E:438:LEU:HA	1.76	0.41
1:C:124:ILE:HD13	1:C:124:ILE:HA	1.95	0.41
1:C:224:HIS:NE2	1:C:266:ARG:HB2	2.35	0.40
1:D:284:CYS:HB2	1:D:323:GLN:HB3	2.01	0.40
1:D:370:ARG:HA	1:D:371:PRO:HD3	1.89	0.40
1:E:276:LYS:NZ	2:E:500:PMP:N4A	2.70	0.40
1:B:7:THR:HA	1:C:255:ALA:HA	2.03	0.40
1:B:342:VAL:HG13	1:C:16:SER:HB2	2.04	0.40
1:D:438:LEU:HD23	1:D:438:LEU:HA	1.92	0.40
1:D:445:LEU:HD23	1:D:445:LEU:HA	1.84	0.40
1:F:262:PHE:CE2	1:F:270:ILE:HD12	2.56	0.40
1:A:99:ARG:O	1:A:103:MET:HG3	2.21	0.40
1:A:163:GLN:HG3	2:A:500:PMP:HNA1	1.87	0.40
1:B:6:VAL:HA	1:C:257:ASP:HB2	2.02	0.40
1:B:410:THR:HA	1:B:418:ILE:O	2.21	0.40
1:C:466:THR:HB	2:C:500:PMP:HNA2	1.87	0.40
1:E:103:MET:HE3	1:F:29:SER:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/466 (98%)	436 (96%)	18 (4%)	1 (0%)	43	71
1	B	462/466 (99%)	436 (94%)	24 (5%)	2 (0%)	30	58
1	C	453/466 (97%)	432 (95%)	21 (5%)	0	100	100
1	D	454/466 (97%)	436 (96%)	18 (4%)	0	100	100
1	E	463/466 (99%)	446 (96%)	17 (4%)	0	100	100
1	F	453/466 (97%)	439 (97%)	13 (3%)	1 (0%)	43	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2740/2796 (98%)	2625 (96%)	111 (4%)	4 (0%)	48	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	GLU
1	F	416	THR
1	B	245	ALA
1	A	412	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	381/390 (98%)	364 (96%)	17 (4%)	24	57
1	B	388/390 (100%)	362 (93%)	26 (7%)	15	40
1	C	379/390 (97%)	362 (96%)	17 (4%)	24	57
1	D	380/390 (97%)	361 (95%)	19 (5%)	22	53
1	E	389/390 (100%)	370 (95%)	19 (5%)	22	53
1	F	379/390 (97%)	370 (98%)	9 (2%)	43	75
All	All	2296/2340 (98%)	2189 (95%)	107 (5%)	23	55

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	30	LYS
1	A	31	ARG
1	A	44	GLN
1	A	124	ILE
1	A	127	SER
1	A	142	ARG
1	A	157	LEU

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Mol	Chain	Res	Type
1	A	177	LEU
1	A	183	ARG
1	A	193	ARG
1	A	200	GLU
1	A	268	LYS
1	A	386	GLU
1	A	417	ASP
1	A	437	LEU
1	A	459	GLN
1	B	9	LEU
1	B	10	ARG
1	B	13	LEU
1	B	21	LYS
1	B	29	SER
1	B	30	LYS
1	B	31	ARG
1	B	34	LEU
1	B	44	GLN
1	B	69	ASP
1	B	127	SER
1	B	131	MET
1	B	142	ARG
1	B	144	ARG
1	B	157	LEU
1	B	177	LEU
1	B	200	GLU
1	B	312	THR
1	B	332	LEU
1	B	344	ASN
1	B	410	THR
1	B	422	ARG
1	B	436	LEU
1	B	437	LEU
1	B	449	SER
1	B	466	THR
1	C	30	LYS
1	C	31	ARG
1	C	44	GLN
1	C	127	SER
1	C	131	MET
1	C	157	LEU
1	C	177	LEU

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Mol	Chain	Res	Type
1	C	183	ARG
1	C	193	ARG
1	C	200	GLU
1	C	315	ILE
1	C	337	GLU
1	C	344	ASN
1	C	437	LEU
1	C	449	SER
1	C	459	GLN
1	C	466	THR
1	D	30	LYS
1	D	31	ARG
1	D	36	GLU
1	D	44	GLN
1	D	114	LYS
1	D	127	SER
1	D	131	MET
1	D	142	ARG
1	D	157	LEU
1	D	177	LEU
1	D	180	ILE
1	D	200	GLU
1	D	221	GLN
1	D	332	LEU
1	D	370	ARG
1	D	398	ARG
1	D	416	THR
1	D	437	LEU
1	D	449	SER
1	E	3	LYS
1	E	4	LYS
1	E	5	GLN
1	E	10	ARG
1	E	31	ARG
1	E	127	SER
1	E	131	MET
1	E	142	ARG
1	E	157	LEU
1	E	177	LEU
1	E	180	ILE
1	E	183	ARG
1	E	200	GLU

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Mol	Chain	Res	Type
1	E	287	VAL
1	E	332	LEU
1	E	370	ARG
1	E	398	ARG
1	E	436	LEU
1	E	437	LEU
1	F	12	GLU
1	F	13	LEU
1	F	31	ARG
1	F	142	ARG
1	F	180	ILE
1	F	200	GLU
1	F	332	LEU
1	F	398	ARG
1	F	437	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	HIS
1	A	216	ASN
1	A	302	ASN
1	A	344	ASN
1	A	459	GLN
1	B	109	HIS
1	B	201	ASN
1	B	216	ASN
1	B	309	GLN
1	B	455	GLN
1	B	459	GLN
1	C	109	HIS
1	C	201	ASN
1	C	216	ASN
1	C	302	ASN
1	C	459	GLN
1	C	461	ASN
1	D	47	ASN
1	D	109	HIS
1	D	216	ASN
1	D	309	GLN
1	D	344	ASN
1	D	455	GLN

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Mol	Chain	Res	Type
1	D	460	GLN
1	E	109	HIS
1	E	216	ASN
1	E	302	ASN
1	E	344	ASN
1	E	459	GLN
1	F	109	HIS
1	F	216	ASN
1	F	344	ASN
1	F	459	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PMP	D	500	-	16,16,16	1.25	2 (12%)	22,23,23	1.87	6 (27%)
2	PMP	E	500	-	16,16,16	1.24	2 (12%)	22,23,23	1.83	7 (31%)
2	PMP	F	500	-	16,16,16	1.41	1 (6%)	22,23,23	1.49	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PMP	B	500	-	16,16,16	1.25	2 (12%)	22,23,23	1.85	6 (27%)
2	PMP	A	500	-	16,16,16	1.24	2 (12%)	22,23,23	1.69	8 (36%)
2	PMP	C	500	-	16,16,16	1.06	2 (12%)	22,23,23	1.49	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PMP	D	500	-	-	0/8/8/8	0/1/1/1
2	PMP	E	500	-	-	4/8/8/8	0/1/1/1
2	PMP	F	500	-	-	0/8/8/8	0/1/1/1
2	PMP	B	500	-	-	2/8/8/8	0/1/1/1
2	PMP	A	500	-	-	2/8/8/8	0/1/1/1
2	PMP	C	500	-	-	0/8/8/8	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	PMP	C2-N1	3.55	1.40	1.33
2	F	500	PMP	C2-N1	3.50	1.40	1.33
2	A	500	PMP	C2-N1	3.15	1.39	1.33
2	B	500	PMP	C2-N1	3.00	1.39	1.33
2	E	500	PMP	C2-N1	2.93	1.39	1.33
2	E	500	PMP	C3-C2	-2.73	1.38	1.41
2	C	500	PMP	C2-N1	2.66	1.38	1.33
2	A	500	PMP	C3-C2	-2.34	1.38	1.41
2	C	500	PMP	C3-C2	-2.27	1.38	1.41
2	D	500	PMP	C3-C2	-2.20	1.38	1.41
2	B	500	PMP	C5-C4	2.02	1.43	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	500	PMP	C4-C4A-N4A	-4.04	93.85	114.85
2	B	500	PMP	C4A-C4-C3	-3.91	113.59	120.22
2	D	500	PMP	C4-C4A-N4A	-3.69	95.66	114.85
2	F	500	PMP	C2A-C2-C3	-3.50	116.70	120.80
2	C	500	PMP	C4-C4A-N4A	-3.42	97.05	114.85
2	D	500	PMP	C2A-C2-C3	-3.28	116.96	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	PMP	C3-C4-C5	3.27	121.70	118.73
2	F	500	PMP	C2A-C2-N1	3.20	123.66	117.64
2	A	500	PMP	C2A-C2-C3	-3.18	117.08	120.80
2	D	500	PMP	O3P-P-O4P	3.14	114.85	106.67
2	E	500	PMP	C2A-C2-C3	-3.12	117.14	120.80
2	D	500	PMP	C3-C4-C5	3.07	121.52	118.73
2	D	500	PMP	C2A-C2-N1	3.07	123.43	117.64
2	B	500	PMP	C4-C4A-N4A	-3.05	99.02	114.85
2	A	500	PMP	C5-C6-N1	-2.76	119.35	123.83
2	E	500	PMP	O4P-P-O1P	-2.69	99.18	106.44
2	F	500	PMP	C3-C4-C5	2.67	121.15	118.73
2	C	500	PMP	C5-C6-N1	-2.66	119.50	123.83
2	B	500	PMP	C4A-C4-C5	2.59	125.46	120.27
2	B	500	PMP	C3-C4-C5	2.43	120.94	118.73
2	E	500	PMP	O3P-P-O4P	2.38	112.88	106.67
2	B	500	PMP	C5-C6-N1	-2.36	120.00	123.83
2	A	500	PMP	O4P-P-O1P	-2.33	100.14	106.44
2	E	500	PMP	O4P-C5A-C5	2.27	113.61	109.36
2	A	500	PMP	C2A-C2-N1	2.25	121.89	117.64
2	E	500	PMP	C5-C6-N1	-2.20	120.26	123.83
2	C	500	PMP	O4P-C5A-C5	2.17	113.43	109.36
2	A	500	PMP	O3P-P-O4P	2.10	112.16	106.67
2	D	500	PMP	C5-C6-N1	-2.08	120.44	123.83
2	B	500	PMP	O2P-P-O4P	2.08	112.09	106.67
2	E	500	PMP	C4A-C4-C3	-2.03	116.79	120.22
2	A	500	PMP	C4-C4A-N4A	-2.01	104.38	114.85
2	A	500	PMP	O3-C3-C4	2.00	123.99	118.18

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	PMP	C3-C4-C4A-N4A
2	B	500	PMP	C5-C4-C4A-N4A
2	E	500	PMP	C5-C4-C4A-N4A
2	A	500	PMP	C3-C4-C4A-N4A
2	E	500	PMP	C4-C5-C5A-O4P
2	E	500	PMP	C3-C4-C4A-N4A
2	E	500	PMP	C6-C5-C5A-O4P
2	A	500	PMP	C5-C4-C4A-N4A

There are no ring outliers.

6 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	PMP	7	0
2	E	500	PMP	6	0
2	F	500	PMP	4	0
2	B	500	PMP	5	0
2	A	500	PMP	2	0
2	C	500	PMP	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	455/466 (97%)	-0.92	0 100 100	4, 14, 42, 62	2 (0%)
1	B	463/466 (99%)	-0.96	0 100 100	4, 14, 40, 66	1 (0%)
1	C	455/466 (97%)	-1.06	1 (0%) 91 89	3, 12, 42, 64	0
1	D	455/466 (97%)	-0.94	0 100 100	4, 14, 43, 65	1 (0%)
1	E	464/466 (99%)	-1.11	1 (0%) 91 89	2, 12, 39, 63	1 (0%)
1	F	455/466 (97%)	-1.03	0 100 100	2, 12, 42, 63	0
All	All	2747/2796 (98%)	-1.00	2 (0%) 92 90	2, 13, 42, 66	5 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	466	THR	2.4
1	E	305[A]	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PMP	D	500	16/16	0.97	0.09	10,20,24,25	11
3	XE	D	501	1/1	0.97	0.08	14,14,14,14	1
3	XE	F	501	1/1	0.97	0.08	22,22,22,22	1
2	PMP	E	500	16/16	0.98	0.08	8,15,20,26	11
2	PMP	F	500	16/16	0.98	0.08	6,15,19,21	11
3	XE	A	501	1/1	0.98	0.08	11,11,11,11	1
3	XE	B	501	1/1	0.98	0.07	18,18,18,18	1
3	XE	C	501	1/1	0.98	0.09	2,2,2,2	1
2	PMP	B	500	16/16	0.98	0.07	6,15,22,24	11
2	PMP	A	500	16/16	0.98	0.07	11,15,20,20	11
3	XE	E	501	1/1	0.99	0.05	7,7,7,7	1
2	PMP	C	500	16/16	0.99	0.07	2,10,15,15	11

6.5 Other polymers [i](#)

There are no such residues in this entry.